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(FILE 'HOME' ENTERED AT 14:35:25 ON 22 DEC 2009)

FILE 'REGISTRY' ENTERED AT 14:35:32 ON 22 DEC 2009

L1 STRUCTURE UPLOADED

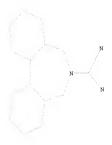
L2 2 S L1

L3 25 S L1 SSS FUL L4 25 S L3 AND CAPLUS/LC

FILE 'CAPLUS' ENTERED AT $14\!:\!37\!:\!13$ ON 22 DEC 2009 L5 13 S L3

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L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr total

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L5 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:845440 CAPLUS

DOCUMENT NUMBER: 151:336783

TITLE: Enantioselective Henry (nitroaldol) reaction catalyzed

by axially chiral guanidines
AUTHOR(S): Ube, Hitoshi; Terada, Masahiro

CORPORATE SOURCE: Department of Chemistry, Graduate School of Science,
Tohoku University, Aoba-ku, Sendai, 980-8578, Japan

SOURCE: Bioorganic & Medicinal Chemistry Letters (2009),

19(14), 3895-3898

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

AB The enantioselective activation of nitroalkanes was attempted on the basis of the complexation between chiral guanidinium and nitronate through two hydrogen bonds. The proposed enantioselective activation was applied to the diastereo- and enantioselective Henry (nitroaldol) reaction of nitroalkanes with aldehydes using axially chiral guanidine bases as the catalyst. Optically active nitroaldol products were obtained in acceptable yields with fairly good enantio- and diastereoselectivities at

low temperature IT 862889-17-6 862889-18-7 862889-19-8 862889-20-1 862889-21-2 862889-22-3 862889-23-4 862889-24-5 1186130-42-6

RL: CAT (Catalyst use); USES (Uses)

(asym. synthesis of nitroalcs. via Henry reaction of nitroalkanes with aldehydes in the presence of axially chiral guanidines)

RN 862889-17-6 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-diphenyl-, (11bR)- (9CI) (CA INDEX NAME)

RN 862889-18-7 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-di-2-naphthalenyl-, (11bR)- (9CI) (CA INDEX NAME)

RN 862889-19-8 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis[3,5-(trifluoromethyl)phenyl]-, (11bR)- (9CI) (CA INDEX NAME)

RN 862889-20-1 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 2,6-bis([1,1'-biphenyl]-4-yl)-3,5-dihydro-, (11bR)- (CA INDEX NAME)

862889-21-2 CAPLUS RN

ouso3-21-2 CAPLUS
4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide,
2,6-bis[3,5-bis(nonafluorobutyl)phenyl]-3,5-dihydro-, (11bR)- (9CI) (CA
INDEX NAME) CN

PAGE 2-A

CF3

RN 862889-22-3 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 2,6-bis[3,5-bis(1,1-dimethylethyl)phenyl]-3,5-dihydro-, (11bR)- (9CI) (CA INDEX NAME)

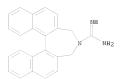
RN 862889-23-4 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis([1,1':3',1''-terphenyl]-5'-yl)-, (11bR)- (CA INDEX NAKE)

- 862889-24-5 CAPLUS 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis[4-(trifluoromethyl)phenyl]-, (11bR)- (9CI) (CA INDEX CN NAME)

- RN
- $1186130-42-6 \quad CAPLUS \\ 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-, (11bR)-1 \\ 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-, (1$ CN (CA INDEX NAME)

10/589,814



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:844930 CAPLUS

DOCUMENT NUMBER: 151:266892

TITLE: Acid-base dual-functional catalysis by axially chiral guanidine in enantioselective [3+2] cycloaddition of maleate to Schiff bases as a precursor of azomethine

vlides

AUTHOR(S): Nakano, Megumi; Terada, Masahiro

CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Tohoku University, Aoba-ku, Sendai, 980-8578, Japan

SOURCE: Synlett (2009), (10), 1670-1674 CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal LANGUAGE: English

AB The enantioselective [3+2] cycloaddn. of maleate with Schiff bases as azomethine ylide precursors was developed using axially chiral guanidine catalysts to provide optically active pyrrolidines. Acid-base dual-functional catalysis by an axially chiral guanidine through double H-bonding interaction is proposed to give the cycloadducts in good vields.

IT 862889-20-1 862889-23-4 921229-45-0

921229-46-1 921229-47-2

RL: CAT (Catalyst use); USES (Uses)

(preparation of pyrrolidines by asym. cycloaddn. of maleate to Schiff bases as azomethine ylide precursors using axially chiral guanidine catalyst)

RN 862889-20-1 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide,

2,6-bis([1,1'-biphenyl]-4-y1)-3,5-dihydro-, (11bR)- (CA INDEX NAME)

RN 862889-23-4 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis([1,1':3',1''-terpheny1]-5'-y1)-, (11bR)- (CA INDEX NAME)

921229-45-0 CAPLUS 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 2,6-bis[3',5'-bis(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]-3,5-dihydro-,(11b8)- (CA INDEX NAME) CN

RN 921229-46-1 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis(5'-phenyl[1,1',3',1''-terphenyl]-4-y1)-, (11bR)- (CA INDEX NAME)

RN 921229-47-2 CAPLUS

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PAGE 1-A

PAGE 2-A

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/589.814

L5 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:527744 CAPLUS

DOCUMENT NUMBER: 151:448018

TITLE: The practical synthesis of double axial chiral

quanidines

AUTHOR(S): Guo, Qun-Sheng; Du, Da-Ming

CORPORATE SOURCE: Beijing National Laboratory for Molecular Sciences

(BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering, College of Chemistry and Molecular Engineering, Peking University, Beijing,

100871, Peop. Rep. China

SOURCE: Letters in Organic Chemistry (2009), 6(3), 197-202 CODEN: LOCEC7; ISSN: 1570-1786

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two novel double axial chiral quanidines were designed according to the concept of double axial chirality. Practical synthetic procedures from (S)-1,1'-binaphthol have been developed. The title compds. were fully characterized by NMR, MS, IR and elemental anal. or HRMS. The two chiral quanidines can be interesting catalysts for asym. catalysis and

preliminary asym. catalytic activity was investigated in Henry reaction and conjugate addition

1190368-96-7P RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(synthesis of double axial chiral guanidines based on binaphthol as catalysts for stereoselective Henry and conjugate addition reactions) RN 1190368-96-7 CAPLUS

CN 7H-Dinaphth[2,3-c:2',3'-e]azepine-7-carboximidamide,

5,9-bis[2-(cyclohexyloxy)-1-naphthalenyl]-6,8-dihydro-, (5S,9S)- (CA INDEX NAME)

10/589,814

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REFERENCE COUNT:

28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/589.814

L5 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:1167756 CAPLUS

DOCUMENT NUMBER: 150:190816

TITLE: Stable and Unstable 6,6- and 5,6- Closed and Open

Adducts of Fullerene C60

AUTHOR(S): Zverev, V. V.; Kovalenko, V. I.

CORPORATE SOURCE: A.E. Arbuzov Institute of Organic and Physical

Chemistry, RAS, Kazan, Russia

SOURCE: Fullerenes, Nanotubes, and Carbon Nanostructures

(2008), 16(5-6), 563-566 CODEN: FNCNAR; ISSN: 1536-383X

PUBLISHER: Taylor & Francis, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

AB DFT/PBE/TZ2P research of total energy of various adducts at variation of 5,6- and 6,6- bond was carried out. On the basis of the anal. of local min., the conclusion on structures stability and instability was drawn. Acyclic and cyclic derivs. containing 4-6-membered rings are established to form the closed adducts only. Thus the [6,6]-closed structures are 15-18 kcal/mol more stable than [5,6]-closed. The [6,6]-closed adducts with strained 3-membered cycles and their [5,6]-open isomers are found to be stable. The anal. of strain energy is accomplished.

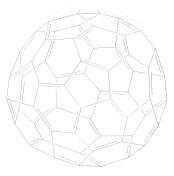
574002-41-8 RL: PRP (Properties)

(stable and unstable 6,6- and 5,6- closed and open adducts of fullerene C60)

RN 574002-41-8 CAPLUS

CN 1'H-[5,6]Fullereno-C60-Ih-[1,9-b]azirine, 1'-(5-nitro-2-pyrimidiny1)- (CA INDEX NAME)





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REFERENCE COUNT:

7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L5 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1069375 CAPLUS

DOCUMENT NUMBER: 148:33366

TITLE: Structure and relative energies of regioisomers and

valence isomers of C60 adducts. HF and DFT study
AUTHOR(S): Zverev, Vladislav V.; Kovalenko, Valeriy I.; Romanova,

Irina P.; Sinvashin, Oleg G.

CORPORATE SOURCE: A.E. Arbuzov Institute of Organic and Physical

Chemistry, Kazan Research Centre, Russian Academy of

Sciences, Kazan, 420088, Russia

SOURCE: International Journal of Quantum Chemistry (2007),

107(13), 2442-2453 CODEN: IJQCB2; ISSN: 0020-7608

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

Fullerene C60 and N-bridged C60NH regioisomeres are investigated by HF and DFT methods with BLYP, B3LYP and PBE functionals at the 6-31G**, 6-311G** and TZ2P levels. Method DFT/PBE/TZ2P, providing the good compliance with exptl. results, is chosen. Cross-sections of potential energy surface of adducts at a variation of 5,6- or 6,6- bonds lengths are investigated. It is shown, that C60C2H4NH and C60H2 are characterized by local min. for [5,6]-closed forms, whereas local min. for [5,6]-open forms are absent. Absence of stable conformations of the [5,6]-closed forms of methanofullerenes and aziridinofullerenes is a consequence of strain energy in three-membered rings. It is shown that relative stability of the regioisomers depends on the lengths of single or double bonds of monoadducts participating in reactions. The coordinated change of relative energies of the open and closed isomers N-bridged mono-(C60NR 1-7) and bis-adducts (C60(NR)2 8-14) is revealed. The [6,6]-closed form is more stable for compds. C60NR (2,3) and cis-1-C60(NR)2 (9,10) (R = Me, Ph), while [5,6]-open and cis-1 [6,6]-open forms are more stable for compds. C60NR (6,7) and cis-1-C60(NR)2 (13,14) (R = C00Me, R* nitropyrimidine), what has been confirmed by experiment. The factors defining relative isomer stability are investigated.

574002-41-8 574002-44-1 944323-06-2

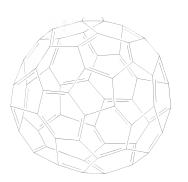
959473-01-9

RL: PRP (Properties)

(structure and relative energies of regioisomers and valence isomers of C60 adducts)

N 574002-41-8 CAPLUS

CN 1'H-[5,6]Fullereno-C60-Ih-[1,9-b]azirine, 1'-(5-nitro-2-pyrimidiny1)- (CA INDEX NAME)



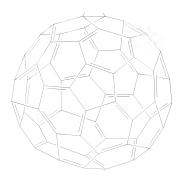
PAGE 2-A

- RN 574002-44-1 CAPLUS
 CN 1'H-[5,6]Fullereno-C60-Ih-[1,9-b]azirine, 1'-(2-pyrimidiny1)- (CA INDEX

NAME)

PAGE 1-A





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RN 944323-06-2 CAPLUS
CN 9a,12a-Diaza-1,9(9a):2,12(12a)-dihomo[5,6]fullerene-C60-1h,
9a,12a-bis(5-methyl-2-pyrimidinyl)- (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 959473-01-9 CAPLUS

CN 9a,12a-Diaza-1,9(9a):2,12(12a)-dihomo[5,6]fullerene-C60-Ih,
9a,12a-di-2-pyrimidinyl- (CA INDEX NAME)

PAGE 1-A

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PAGE 2-A

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD

(1 CITINGS)

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L5 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:110756 CAPLUS

DOCUMENT NUMBER: 147:188674

TITLE: Synthesis and unusual electrochemical properties of

nitropyrimidine-substituted

diazadihomo(C60-Ih)[6,6]fullerene
AUTHOR(S): Romanova, Irina P.; Yusupova, Gulshat G.; Larionova,

Olga A.; Nafikova, Adilya A.; Yakhvarov, Dmitry G.; Zverev, Vladislav V.; Efremov, Yury Ya.; Sinyashin, Oleg G.

CORPORATE SOURCE: A. E. Arbuzov Institute of Organic and Physical

Chemistry, Kazan Scientific Centre of the Russian Academy of Sciences, Kazan, 420088, Russia

SOURCE: Mendeleev Communications (2006), (6), 309-311

CODEN: MENCEX; ISSN: 0959-9436
PUBLISHER: Russian Academy of Sciences

PUBLISHER: Russian DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:188674

AB A bisadduct regioisomer with two open transannular [6,6]-bonds was synthesized by the cycloaddn, reaction of C60 and

2-azido-5-nitropyrimidine.

IT 574002-41-8

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

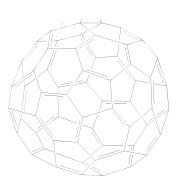
(failed cycloaddn. reaction with 2-azido-5-nitropyrimidine and

electroredn.; synthesis of nitropyrimidine-substituted diazadihomo(C60-Ih)[6,6]fullerene by cycloaddn. of

2-azido-5-nitropyrimidine with C60 and its electroredn.)

RN 574002-41-8 CAPLUS

CN 1'H-[5,6]Fullereno-C60-Ih-[1,9-b]azirine, 1'-(5-nitro-2-pyrimidinyl)- (CA INDEX NAME)



PAGE 2-A

II 944323-06-2P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT

(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (preparation, structural characterization, and electroredn.; synthesis of nitropyrimidine-substituted diazadihomo(C60-Ih)[6,6]fullerene by cycloaddn. of 2-azido-5-nitropyrimidine with C60 and its electroredn.)

RN 944323-06-2 CAPLUS CN 9a,12a-Diaza-1,9(9a):2,12(12a)-

9a,12a-Diaza-1,9(9a):2,12(12a)-dihomo[5,6]fullerene-C60-Ih, 9a,12a-bis(5-methyl-2-pyrimidinyl)- (CA INDEX NAME)

N N

PAGE 2-A

OS.CITING REF COUNT:

REFERENCE COUNT:

- 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
- 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:1250291 CAPLUS

DOCUMENT NUMBER: 146:184341

TITLE: Axially Chiral Guanidine as Highly Active and

Enantioselective Catalyst for Electrophilic Amination

of Unsymmetrically Substituted 1,3-Dicarbonyl

Compounds

AUTHOR(S): Terada, Masahiro; Nakano, Megumi; Ube, Hitoshi

CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Tohoku University, Sendai, 980-8578, Japan

SOURCE: Journal of the American Chemical Society (2006),

128(50), 16044-16045

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: Journal English

OTHER SOURCE(S): CASREACT 146:184341

GI

AB Nonracemic axially chiral guanidines such as dinaphthoazepineamidine I are prepared; I is an effective catalyst for the enantioselective addition of β-oxoesters and a 1,3-diketone to di-tert-Bu azodicarboxylates to yield α-hydrazino-β-oxoesters and an α-hydrazino-b-oxoesters and an α-hydrazino-b-oxoesters and an α-hydrazino-b-oxoesters and an an analysis of the twelve examples give products in 83-98% ee). For example, stirring Et 2-oxocyclopentanecarboxylate and di(tert-butyl)

azodicarboxylate in THF in the presence of 0.05 mol% I for 4 h at -60° provides II [Boc = Me3COC(:0)] in quant. yield and in 97% ee. Dinaphthoazepineamidine catalysts with other substituted Ph groups at the 3,3'-positions give addition/amination products in lower rates and enantioselectivities. I is prepared in six steps from (R)-2,2'-dimethyl-3,3'-binaphthalenediol ditrifiate, 4-methoxyphenylboronic acid, and 3,5-di(tert-butyl)phenylboronic acid. The absolute stereochemistries of three of the products are determined by their conversions to known oxazolidinones.

IT 862889-20-1P 862889-23-4P 921229-46-1P

921229-47-2P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(dinaphthoazepineamidine prepared and tried as a catalyst for the enantioselective addition of Et 2-oxocyclopentanecarboxylate to di(tert-butyl) azodicarboxylate to yield a nonracemic $\alpha\text{-hydrazino-}\beta\text{-ketoester})$

RN 862889-20-1 CAPLUS

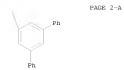
CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide,

2,6-bis([1,1'-biphenyl]-4-yl)-3,5-dihydro-, (11bR)- (CA INDEX NAME)

RN 862889-23-4 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis([1,1':3',1''-terphenyl]-5'-yl)-, (11bR)- (CA INDEX NAME)

921229-46-1 CAPLUS
4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide,
3,5-dihydro-2,6-bis(5'-phenyl[1,1',3',1''-terphenyl]-4-y1)-, (11bR)- (CA
INDEX NAME) CN



- RN 921229-47-2 CAPLUS

921229-45-0P

CN

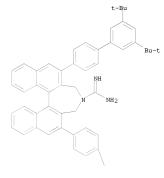
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

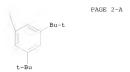
(preparation of a dinaphthoazepineamidine and its use as a catalyst for the enantioselective addition of 1,3-dicarbonyl compds. to azodicarboxylates to yield α -hydrazino- β -oxoesters and an α-hydrazino-β-diketone)

RN 921229-45-0 CAPLUS

4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide,
2,6-bis[3',5'-bis(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]-3,5-dihydro-, (11bR) - (CA INDEX NAME)

PAGE 1-A





OS.CITING REF COUNT:

37

60 THERE ARE 60 CAPLUS RECORDS THAT CITE THIS RECORD (61 CITINGS)

REFERENCE COUNT:

THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/589.814

L5 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:796909 CAPLUS

DOCUMENT NUMBER: 147:166276

TITLE: Synthesis, electrochemical properties, and thermal

transformations of

1-(5-nitro-2-pyrimidinyl)[60]fullereno[1,2-b]aziridine AUTHOR(S): Romanova, I. P.; Yusupova, G. G.; Larionova, O. A.;

Balandina, A. A.; Latypov, Sh. K.; Zverev, V. V.;

Yakhvarov, D. G.; Rusinov, G. L.; Sinyashin, O. G. A. E. Arbuzov Institute of Organic and Physical CORPORATE SOURCE:

Chemistry, Kazan Research Center, Russian Academy of Sciences, Kazan, 420088, Russia

SOURCE: Russian Chemical Bulletin (2006), 55(3), 502-506

CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER . Springer DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:166276

The reaction of fullerene C60 with 2-azido-5-nitropyrimidine afforded 1-(5-nitro-2-pyrimidinyl)[60]fullereno[1,2-b]aziridine, whose electrochem. reduction proceeds more easily than the reduction of non-modified C60.

574002-41-8P

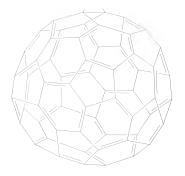
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of [(nitro)pyrimidinyl]fullereno[1,2-b]aziridine derivs. and study of their electrochem, properties and thermal transformation)

574002-41-8 CAPLUS RN

CN 1'H-[5,6]Fullereno-C60-Ih-[1,9-b]azirine, 1'-(5-nitro-2-pyrimidinyl)- (CA INDEX NAME)



PAGE 2-A



- OS.CITING REF COUNT: 3
- REFERENCE COUNT:
- THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
- THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT 21

L5 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:902859 CAPLUS

DOCUMENT NUMBER: 143:229737

TITLE: Preparation of optically active bi-aryl guanidine

compounds as catalysts for asymmetric reactions
INVENTOR(S): Terada, Masahiro; Ube, Hitoshi; Yokoyama, Shiqeko;

Shimizu, Hideo

PATENT ASSIGNEE(S): Takasago International Corporation, Japan

SOURCE: PCT Int. Appl., 60 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

					KIND		DATE		APPLICATION NO.						DATE		
W	WO 2005077908				A1 20050825			WO 2005-JP1943						20050209			
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GO,	GW,	ML,
		MR,	NE,	SN,	TD,	TG											
US 20080154036					A1		20080626 US 2006-589814								20060921		
PRIORITY APPLN. INFO.: JP 2004-41181 A													A 2	20040218			
WO 2005-JP1943 W													7 2	0050	209		
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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE(S): MARPAT 143:229737 GI

AB Guanidine compds. which have a bi-aryl skeleton represented by the following general formula (I) [wherein R1-R3 = H, each (un)substituted hydrocarbon or heterocyclic group; R4, R15 = H, H0, CO2H, acyl, each (un)substituted hydrocarbon, heterocyclic, alkoxy, aryloxy,

alkoxycarbonyl, aryloxycarbonyl, carbamoyl, alkylthiocarbonyl, arylthiocarbonyl, arkylthio, arylthio, or aminio group, or substituents silyl group, or in any combination of R1 to R15, these substituents may together bind with each other to form a ring; X1-X8 = carbon or nitrogen atom, with the provise that each of X1 to X8 has no substituent when it is nitrogen] are prepared The above quanidine compds. are useful as catalysts for a variety of asym. reactions such as asym. nucleophilic addition reaction, asym. Michael addition reaction, asym. epoxidn., and asym. nitro aldol reaction (Henry reaction). Thus, 0.48 g quanidine hydrochloride was neutralized by Amberlite IRA-400 (OH-) and eluted out by ethanol to give ethanol solution of quanidine (5 mL) which was added to a solution of 0.3 g (8)-3,3'-diphenyl-2,2'-bis(bromomethyl)-1,1'-binaphthyl in 5 mL THE. The resulting mixture was heated at 50° and treated with 1 M aqueous HCl

workup

and silica gel chromatog., 80% 4,5-dihydro-3H-dinaphth[2,1-c:1',2'-e]azepine-4-carboxamidine derivative (II) (R = Ph). A mixture of guanidine compound II [R = 3,5-bis(trifluoromethyl)phenyl] (7.6 mg), 1 mL THF, and 20.3 μ L was cooled to -40%, treated dropwise with 108 μ L nitromethane, and stirred 23 h, and quenched by adding 1 M HC1/MeOH solution to give, after workup and silica gel chromatog., 95%

(S)-2-nitro-1-phenylethanol (46% ee) (asym. nitro aldol reaction).

IT 862889-17-6P 862889-18-7P 862889-19-8P 862889-20-1P 862889-21-2P 862889-22-3P 862889-23-4P 862889-24-5P 862889-25-6P

862889-26-7P 862889-27-8P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (preparation of optically active quanidine compds. as catalysts for asym.

reactions)

RN 862889-17-6 CAPLUS
CN 4H-Dinaphth[2,1-c.1',2'-e]azepine-4-carboximidamide,
3,5-dihvdro-2,6-dibhenvl-, (1lbR)- (9CI) (CA INDEX NAME)

RN 862889-18-7 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-di-2-naphthalenyl-, (11bR)- (9CI) (CA INDEX NAME)

RN 862889-19-8 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis[3,5-(trifluoromethyl)phenyl]-, (11bR)- (9CI) (CA INDEX NAME)

RN 862889-20-1 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 2,6-bis([1,1'-biphenyl]-4-yl)-3,5-dihydro-, (11bR)- (CA INDEX NAME)

- 862889-21-2 CAPLUS RN
- ouso3-21-2 CAPLUS
 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide,
 2,6-bis[3,5-bis(nonafluorobutyl)phenyl]-3,5-dihydro-, (11bR)- (9CI) (CA
 INDEX NAME) CN

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CF3

RN 862889-22-3 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 2,6-bis[3,5-bis(1,1-dimethylethyl)phenyl]-3,5-dihydro-, (11bR)- (9CI) (CA INDEX NAME)

RN 862889-23-4 CAPLUS

CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis([1,1':3',1''-terphenyl]-5'-yl)-, (11bR)- (CA INDEX NAKE)

862889-24-5 CAPLUS 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis[4-(trifluoromethyl)phenyl]-, (11bR)- (9CI) (CA INDEX CN NAME)

862889-25-6 CAPLUS RN

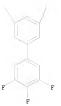
CN 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 2,6-bis[3,5-bis(trimethylsilyl)phenyl]-3,5-dihydro-, (11bR)- (9CI) (CA INDEX NAME)

862889-26-7 CAPLUS 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 3,5-dihydro-2,6-bis[3,3'',5,5''-tetrakis(trifluoromethyl)[1,1':3',1''-CN terphenyl]-5'-yl]-, (11bR)- (9CI) (CA INDEX NAME)

PAGE 2-A

- RN
- 862889-27-8 CAPLUS 4H-Dinaphth[2,1-c:1',2'-e]azepine-4-carboximidamide, 2,6-bis(3,3'',4,4'',5,5''-hexafluoro[1,1':3',1''-terphenyl]-5'-yl)-3,5-dihydro-, (1lbR)- (9C1) (CA INDEX NAME) CN

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- OS.CITING REF COUNT:
- REFERENCE COUNT:
- THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
- 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:30561 CAPLUS

DOCUMENT NUMBER: 141:225438

TITLE: Reaction of fullerene C60 with 2-azido-4,6-diphenylpyrimidine

AUTHOR(S): Romanova, I. P.; Yusupova, G. G.; Yakhvarov, D. G.;

Larionova, O. A.; Mochul skaya, N. N.; Sidorova, L. P.; Charushin, V. N.; Zverev, V. V.; Sinyashin, O. G.

CORPORATE SOURCE: A. E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Research Center of the Russian

Academy of Sciences, Kazan, 420088, Russia
SOURCE: Russian Chemical Bulletin (Translation of Izvestiya

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2003), 52(10),

2171-2174

CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:225438

AB The first representative of the pyrimidine-substituted

[60]fullereno[1,2-b]aziridines was synthesized by the reaction of fullerene C60 with 2-azido-4,6-diphenylpyrimidine.

2-(Azahomo[60]fullereno)-4,6-diphenylpyrimidine was found to be formed as a byproduct. The electrochem. and MO properties of the adducts were studied.

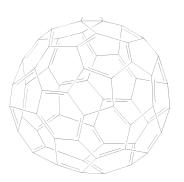
T 745794-90-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of substituted fullerenoaziridines via reaction of fullerene C60 with azidodiphenylpyrimidine and their electrochem. and MO properties)

RN 745794-90-5 CAPLUS

CN 1'H-[5,6]Fullereno-C60-Ih-[1,9-b]azirine, 1'-(4,6-diphenyl-2-pyrimidinyl)(9CI) (CA INDEX NAME)





10

PAGE 2-A

REFERENCE COUNT:

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:125843 CAPLUS

DOCUMENT NUMBER: 139:164691

TITLE: Reactions of [60]fullerene with 2-azidopyrimidines AUTHOR(S): Romanova, I. P.; Kalinin, V. V.; Nafikova, A. A.; Yakhvarov, D. G.; Zverev, V. V.; Kovalenko, V. I.;

Rusinov, G. L.; Plekhanov, P. V.; Charushin, V. N.;

Sinyashin, O. G. CORPORATE SOURCE: A. E. Arbuzov In:

A. E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Research Center of the Russian

Academy of Sciences, Kazan, 420088, Russia
SOURCE: Russian Chemical Bulletin (Translation of Iz

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2003), 52(1),

173-178 CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:164691

AB The reaction of [60]fullerene with 2-azido-5-nitropyrimidine or 2-azidopyrimidine affords fullerenoimidazopyrimidines, whose electron affinity is higher than that of non-modified (60. Formation enthalpy, relative energy, electron affinity, reduction potential of these adducts thus prepared were determined through the AMI (MO) and PM3 (MO) methods and obtained from the first wave potentials of the electrochem. reduction of fullerene-C60

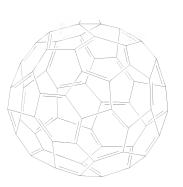
and its derivs. IT 574002-44-1

RL: PRP (Properties)
(reaction of [60]fullerene with 2-azidopyrimidines)

RN 574002-44-1 CAPLUS

CN 1'H-[5,6]Fullereno-C60-Ih-[1,9-b]azirine, 1'-(2-pyrimidiny1)- (CA INDEX NAME)





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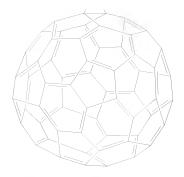
IT 574002-41-8P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(reaction of [60]fullerene with 2-azidopyrimidines)

- RN 574002-41-8 CAPLUS
- CN 1'H-[5,6]Fullereno-C60-Ih-[1,9-b]azirine, 1'-(5-nitro-2-pyrimidiny1)- (CA INDEX NAME)



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- OS.CITING REF COUNT:
- REFERENCE COUNT: 14
- 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
 - 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/589.814

L5 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:7348 CAPLUS
DOCUMENT NUMBER: 112:7348
ORIGINAL REFERENCE NO.: 112:1439a,1442a

TITLE: Synthesis and biological activity of

dibenz[c,e]azepines

AUTHOR(S): Aboul-Enein, Hassan Y.; Ibrahim, Said E.; Khalifa, M. CORPORATE SOURCE: Coll. Pharm., King Saud Univ., Rivadh, 11451, Saudi

Arabia

SOURCE: Drug Design and Delivery (1988), 4(1), 27-33

CODEN: DDDEEJ; ISSN: 0884-2884

DOCUMENT TYPE: Journal LANGUAGE: English

AB Synthesis and pharmacol. screening of 68 dibenz[c,e]azepines are described. All were inactive as antidepressant agents, but two compds. showed good anticonvolvant activity. The structure-activity relationships

of this class of compds. are discussed. IT 124214-32-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydride reduction of, dibenzazepine by)

RN 124214-32-0 CAPLUS

CN 5H-Dibenz[c,e]azepine-5,7(6H)-dione, 6-(1H-1,2,4-triazol-5-yl)- (CA INDEX NAME)

IT 124214-29-5P 124214-50-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 124214-29-5 CAPLUS

CN 5H-Dibenz[c,e]azepine-5,7(6H)-dione, 6-(2-pyrimidinyl)- (CA INDEX NAME)

- RN 124214-50-2 CAPLUS
- CN 5H-Dibenz[c,e]azepine, 6,7-dihydro-6-(1H-1,2,4-triazol-5-y1)- (CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L5 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1983:125269 CAPLUS

DOCUMENT NUMBER: 98:125269

ORIGINAL REFERENCE NO.: 98:19071a,19074a

TITLE: A carbon-13 NMR assignment study of certain 6-substituted dibenz[c,e]azepine-5,7-dione

AUTHOR(S): Ibrahim, Said E.; Aboul-Enein, Hassan Y.; Khalifa, M.

CORPORATE SOURCE: Coll. Pharm., King Saud Univ., Riyadh, Saudi Arabia

SOURCE: Spectroscopy Letters (1982), 15(7), 575-81

CODEN: SPLEBX; ISSN: 0038-7010

DOCUMENT TYPE: Journal

LANGUAGE: English

CO2H CO2H Ι

- The natural abundance 13C NMR of I and II (R = m-CF3C6H4, 2-pyridyl, morpholino, 1,2,4-triazol-3-yl) are observed using the Fourier transform technique. The 13C chemical shifts are assigned on the basis of chemical shift theory, the observed signal multiplicity in the single frequency off-resonance decoupled spectra, and comparison with the chemical shifts of the model compds.
- 84679-66-3 RL: PRP (Properties)
- (carbon-13 NMR of) RN 84679-66-3 CAPLUS
- CN 5H-Dibenz[c,e]azepine-5,7(6H)-dione, 6-(3H-1,2,4-triazol-3-y1)- (CA INDEX NAME)